

## Petrus (Peter) H. Zwart

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CONTACT INFORMATION	1 Cyclotron Road ALS, Bldg 6, Room 2134 Berkeley Nat. Laboratories Berkeley, 94720 CA, USA	<i>cell phone:</i> +1 510 289 9246 <i>work phone:</i> +1 510 486 4214 <i>work fax:</i> +1 510 486 5664 <i>email:</i> PHZwart@lbl.gov
STATUS	Date and place of birth Sex Marital Status Nationality	May 10, 1976, Anna Paulowna, The Netherlands Male Married Dutch. In possession of a PIO card since 2007.
RESEARCH INTERESTS	The application of computational techniques on the interface between chemistry, biology, physics and bioinformatics in the pursuit of understanding complex biological systems on a molecular level.	
EDUCATION AND RESEARCH	September 1994 – August 1999	M.Sc. Chemistry, University of Amsterdam, Faculty of Chemistry, Laboratory of Crystallography.
	November 1997 – February 1998	Research project at the European Molecular Biology Laboratory (EMBL) in the group of Dr. V.S. Lamzin on the structure solution and refinement of SS-LADH.
	December 1998 – March 1999	Research project at the European Synchrotron Radiation Facility (ESRF) in the group of Dr. H. Graafsma on the crystal structure of deuterated Potassium Phosphate in a static electric field.
	September 1999 – August 2003	PhD-student at European Molecular Biology Laboratory (EMBL), Hamburg Outstation, in the group of Dr. V.S. Lamzin.  Home institute and supervisor: University of Amsterdam, Prof. Dr. H. Schenk. Defense date: December 17, 2003.
	September 2003 – October 2003	Postdoctoral fellow at European Molecular Biology Laboratory (EMBL), Hamburg Outstation, in the group of Dr. V.S. Lamzin.
	February 2004 – November 2005	Postdoctoral fellow with SAIC-Frederick Inc. in the group of Dr. Z. Dauter located at the NSLS, Brookhaven National Laboratories, Upton NY, USA
	November 2004 – March 2005	Postdoctoral fellow with SAIC-Frederick Inc. in the group of Dr. Z. Dauter located at the Argonne National Laboratories, Argonne, IL, USA
	March 2005 – Februari 2007	Postdoctoral fellow in the group of Dr. Adams, Lawrence Berkeley National Laboratories, Berkeley, CA, USA
	March 2007 – Present	Research Scientist in the Advanced Light Source, Berkeley National Laboratories, CA, USA.

AWARDS,  
FELLOWSHIPS  
GRAND PROPOSALS

June 1999	EMBL Fellowship to carry out PhD-research in the group of Dr. Lamzin.
October 2000	Unilever Research Price for undergraduate work.
October 2008	LDRD funded proposal for the development of software in biological small angle scattering. (with A. Hexemer & P. Adams; 100K USD )
October 2009	LDRD funded proposal for the development of software in biological small angle scattering. (with A. Hexemer & P. Adams; 100K USD )

PUBLICATIONS

**Zwart, P.H.**, Grosse-Kunstleve, R.W. & Adams, P.D. (2009). Handling of twinned data in the PHENIX software package. *in preparation*.

Liu, H., **Zwart, P.H.** (2009). The Small Angle Scattering Toolbox. *in preparation*

Chuang, C.K., Rockel, B., Seyit, G., Walian, P., Schonegge, A., Peters, J., **Zwart, P.H.**, Baumeister, W., Jap, B.K (2009). Hybrid Molecular Structure of the Giant Protease Tripeptidyl Peptidase II. *Submitted to Cell*.

Terwilliger T.C., Adams P.D., Read R.J., McCoy A.J., Moriarty N.W., Grosse-Kunstleve R.W., Afonine P.V., **Zwart P.H.**, Hung L.W. (2009). Decision-making in structure solution using Bayesian estimates of map quality: the PHENIX AutoSol wizard. *Acta Cryst* **D65**, 582-601.

Sauter N.K. & **Zwart P.H.** (2009). Autoindexing the diffraction patterns from crystals with a pseudotranslation. *Acta Cryst.* **D65**, 553-559.

**Zwart, P.H.**, Afonine, P.V., Grosse-Kunstleve, R.W., Hung, L-W., Ioerger, T.R., McCoy, A.J., McKee, E., Moriarty, N.W., Read, R.J., Richardson, D., Richardson, J., Sacchettini, J.C., Sauter, N.K., Storoni, L.C., Terwilliger, T.C. & Adams, P.D. (2008). Automated structure solution with the Phenix suite. Chapter in: *Methods in molecular biology*, **426**, 419–436.

Terwilliger, T.C., Grosse-Kunstleve, R.W., Afonine, P.V., Moriarty, N.W., **Zwart, P.H.**, Hung, L.-W, Read, R.J. and Adams, P.D. (2008). Iterative model building, structure refinement and density modification with the PHENIX AutoBuild wizard. *Acta Cryst.* **D64**, 61–69.

**Zwart, P.H.**, Grosse-Kunstleve, R.W., Lebedev, A., Murshudov, G. & Adams, P.D. (2008). Surprises and pitfalls arising from (pseudo)symmetry. *Acta Cryst.* **D64**, 99–107.

Terwilliger, T.C., Grosse-Kunstleve, R. , Afonine, P.V., Adams, P.D., Moriarty, N.W., **Zwart, P.H.** , Read, R.J., Turk, D. & Hung, L-W. (2007). Interpretation of ensembles created by multiple iterative rebuilding of macromolecular models, *Acta Cryst* **D63**, 597–610.

**Zwart, P.H.** (2005). Anomalous signal indicators in protein crystallography, *Acta Cryst.* **D61**, 1437–1448.

**Zwart, P.H.**, Langer G.G. & Lamzin, V.S. (2004). Modeling Bound ligands in protein crystal structures, *Acta Cryst.* **D60**, 2230–39

**Zwart, P.H.**, Banumathi, S. , Dauter, M. & Dauter, Z. (2004). Radiation-damage-induced phasing with anomalous scattering: substructure solution and phasing, *Acta Cryst.* **D60**, 1958–63.

Banumathi, S., **Zwart, P.H.**, Ramagopal, U.A., Dauter, M. & Dauter Z. (2004). Structural effects of radiation damage and its potential for phasing, *Acta Cryst.* **D60**, 1085–93.

**Zwart, P.H.** & Lamzin, V.S. (2004). The influence of positional errors on the Debye effects, *Acta Cryst.* **D60**, 220–6.

**Zwart, P.H.** (2003). Error Estimation and Pattern Recognition Techniques in Protein Crystallography. (PhD Thesis).

**Zwart, P.H.** & Lamzin, V.S. (2003). Distance distributions and electron density characteristics of protein models, *Acta Cryst.* **D59**, 2104–13..

Morris, R.J., **Zwart, P.H.**, Cohen, S., Fernandez, F.J., Kakaris M., Kirillova, O., Vonnrhein, C., Perrakis, A. & Lamzin, V.S. (2003). Breaking good resolutions with ARP/wARP, *J. Synch. Rad.* **11**, 56–9.

Lorentzen, E., Pohl, E., **Zwart, P.**, Stark, A., Russell, R.B., Knura, T., Hensel, R., Siebers, B. (2003). Crystal structure of an archaeal class I aldolase and the evolution of ( $\beta\alpha$ )<sub>8</sub> barrel proteins. *J Biol Chem.* **278**, 47253–60

Pegasova, T.V., **Zwart P.H.**, Koroleva O.V., Stepanova E.V., Rebrikov D.V. & Lamzin V.S. (2003). Crystallization and preliminary X-ray analysis of a four-copper laccase from *Coriolus hirsutus*. *Acta Cryst.* **D59**, 1459–61.

Van Langevelde, A., Van Malssen, K., Driessen, R., Goubitz, K., Hollander, F., Peschar R., **Zwart P.**, & Schenk H. (2000). Structure of CnCn+2Cn-type (n = even) beta'-triacylglycerols. *Acta Cryst.* **B56** 1103–11.

Adolph H.W., **Zwart, P.**, Meijers, R., Hubatsch, I., Kiefer, M., Lamzin, V., Cedergren-Zeppezauer, E. (2000). Structural basis for substrate specificity differences of horse liver alcohol dehydrogenase isozymes. *Biochemistry* **39** 12885–97.

#### NON PEER-REVIEWED ARTICLES

Banumathi, S., **Zwart, P.H.**, Dauter, M., Dauter, Z., (2004) Structural effects of radiation damage and its potential for phasing, *National Synchrotron Light Source Science Highlights*, November 5, 2004. (<http://www.nsls.bnl.gov/newsroom/science/2004/11-Dauter.htm>).

**Zwart, P.H.**, Grosse-Kunstleve, R.W. & Adam, P.D. (2005) Characterization of X-ray data sets. *CCP4 Newsletter* No. 42.

**Zwart, P.H.**, Grosse-Kunstleve, R.W. & Adam, P.D. (2005) Xtriage and Fest: automatic assessment of X-ray data and substructure structure factor estimation. *CCP4 newsletter* No. 43

**Zwart, P.H.**, Grosse-Kunstleve, R.W. & Adam, P.D. (2006) Exploring Metric Symmetry. *CCP4 newsletter* No. 44

Morton, S., Glossinger, J., Smith-Baumann, A., McKean, J.P., Trame, C., Dickert, J., Rozales, A., Dauz, A., Taylor, J., **Zwart, P.**, Duarte, R., Padmore, H., McDermott, G. & Adams, P. (2007). Technical Report: Recent Major Improvements to the ALS Sector 5 Macromolecular Crystallography Beamlines, *Synchrotron Radiation News* **20**, 23–30.

NOTEWORTHY  
ACKNOWLEDGMENTS

Kim, J., Sitaraman, S., Hierro, A., Beach, B.M., Odorizzi, G. & Hurley J.H. (2005). Structural Basis for Endosomal Targeting by the Bro1 Domain. *Developmental Cell* 8,937–47.

Salameh, M.A., Soares, A., Hockla, A., Radisky, E.S. (2007), Structural basis for accelerated cleavage of bovine pancreatic trypsin inhibitor (BPTI) by human mesotrypsin. *J. Biol. Chem.* epub ahead of print, Dec 12, 2007.

Faham, S., Wanatabe, A., Mercado Besserer, G., Cascio, D., Specht, A., Hirayama, B.A., Wright, E.M. & Abramson, J. (2008), The crystal structure of a sodium galactose transporter reveals mechanistic insights into a Na<sup>+</sup> / sugar symport. *Science* 321,810-814.

ORAL PRESENTATIONS

*Coordinate Error estimation of a set of free atoms*, XIXth International Union of Crystallography Conference and General Assembly, August 6–15, 2002, Geneva, Switzerland (**Invited Speaker**).

*Automated Ligand building in ARP/wARP*, Current Trends in Structure Aided Drug Design, May 22–24, 2003, Lund, Sweden (**Invited Speaker**).

*Ligand Fitting*, CCP4 Study Weekend 2004, January 4–5, 2004, Leeds, United Kingdom (**Invited Speaker**).

*Anomalous signal indicators in protein crystallography*, January 21, 2005, University of Madras (host: Prof. Dr. D. Velmurugan), Chennai, India.

*Anomalous signal indicators in protein crystallography*, CCP4 workshop on computational crystallographic methods, March 15–20, 2005, IISc, Bangalore, India (**Invited speaker**).

*Radiation damage induced phasing with anomalous scattering*, ACA annual meeting, May 28 – June 2, 2005, Orlando, USA (**Invited speaker**).

*Data quality assessment with Xtriage & Automated structure solution with PHENIX*, National University of Singapore (host: Prof. Dr. K. Swaminathan), June 30, 2005, Singapore.

*First aid and Pathology; Data quality assessment with Xtriage* International Symposium on Recent Trends in Macromolecular Structure and Function, January 18–20, 2006, Chennai, Tamil Nadu, India (**Invited speaker**; Member of organizing committee).

*Data quality assessment with Xtriage*, Gordon research conference on Diffraction Methods in Structural Biology, June 16–21, 2006, Lewiston, USA.

*General Pathologies*, CCP4 Study Weekend, Januari 4–6, 2007, Leeds, United Kingdom (**Invited speaker**)

*Twinning and PHENIX*, ACA anual meeting, July 21–26, 2007, Salt Lake City, UT, USA.

*Twinning and PHENIX*, Phenix User Meeting 2008, March 27–28, 2008, LBL, Berkeley, CA, USA

*Crystallography on a fault line*, April 10, 2008, Swiss Light Source, Villigen, Switzerland

TEACHING AND  
TUTORIALS

Tutor at beam line X9B during the NSLS *Rapidata 2004* course, April 25–30, 2004, NSLS, Brookhaven, NY, USA.

Tutor in CCP4 workshop on computational crystallographic methods, March 15–20, 2005, IISc, Bangalore, India.

*Automated structure solution with PHENIX*, ALS user meeting workshop, October 20–22, 2005, ALS, Berkeley, USA.

*Data quality assessment with Xtriage*, International Conference on Structural Genomics, October 19–21, 2006, Riken, Yokohama, Japan.

Tutor at beam line X3A during the NSLS *Rapidata 2007* course, April 22–27, 2007, NSLS, Brookhaven, NY, USA.

*Introduction to structure solution and refinement*, SSRL Structural Molecular Biology Summer School, September 9–14, 2007, Stanford Synchrotron Research Laboratory, Menlo Park, CA, USA

Tutor in the hands on sessions at the Phenix User Meeting 2008, March 27–28, 2008, LBL, Berkeley, CA, USA.

Tutor in the EMBO workshop ‘Structure determination of macromolecules’, September 14–20, 2008 in Synchrotron Soleil, France.

Speaker in the Como Crystallography school, September 29 – October 3rd, 2008, Como, Italy.

Speaker and organizer of twinning workshop, August 25, 2009, Toronto, Canada

Tutor, Speaker and organizer of Phenix User Meeting 2009, October 8–9, 2009, LBL, Berkeley, CA, USA

POSTER  
PRESENTATIONS

*Modeling bound ligands in protein crystal structures*. Gordon Research Conference on Diffraction Methods in Structural Biology, June 11–16, Lewiston, USA.

*Radiation-damage induced phasing with anomalous scattering*. Gordon Research Conference on Diffraction Methods in Structural Biology, June 11–16, Lewiston, USA.

*Characterizing X-ray data sets with Xtriage*. Gordon research conference on Diffraction Methods in Structural Biology, June 16–21, Lewiston, USA.

ORGANISATION  
COMMITTEES

*International Symposium on Recent Trends in Macromolecular Structure and Function* January 18–20, 2006, Chennai, Tamil Nadu, India.

*ALS user meeting session: Design and function of Protein Nanostructures*, October 5th, 2007, Berkeley, CA, USA.

*Phenix User Meeting 2008 (PhUMe08)* March 27–28, 2008, Berkeley, CA., USA.

*ALS user meeting session: Recent advances in the automation of protein crystallography* October 14, 2008, Berkeley, CA, USA.

*ACA workshop: Twinning* June 2009, Toronto, Canada.

*Phenix User Meeting 2009 (PhUMe09)* october 8 –9, 2009, Berkeley, CA., USA.

SKILLS

**Languages**

Dutch: Mother tongue, English: Fluent, German: Good; Tamil: Basic

**Operating systems**

working knowledge of UNIX, LINUX, Windows and Mac OSX

**Programming**

Working knowledge of C++ and python, Limited knowledge of Fortran, Java and PHP.  
Co-developer of the open source CCTBX crystallographic libraries (<http://cctbx.sf.net>).  
Limited experience with the open source Clipper libraries for crystallographic computing.

Principle developer of the Small Angle Scattering Toolbox (<http://sastbx.sf.net>)

**Scientific Software**

Experience with most crystallographic software, notably PHENIX, HKL2000, BEST ARP/wARP, Solve/Resolve, SHARP, SHELXC/D/E, SnB, CCP4.

Co-author of PHENIX software and ARP/wARP. Principle Investigator in SASTBX project.

**Synchrotron experience**

Performed experiments on most crystallographic beam lines at the EMBL-Hamburg outstation.

Performed user support and experiments on NSLS crystallography beam line X9B.

Performed experiment on SERCAT 22-BM APS crystallography beam line.

Performed static and time resolved measurements on the ALS SAXS beam line 7.3.3.

Performed experiments and user support on sector 8.2.n ALS crystallography beam lines.

Beamline scientist at the Berkeley Center for Structural Biology (BCSB, <http://bcsb.lbl.gov>) responsible for 2 fixed (ALS BL5.0.1. and ALS BL5.0.3.) wavelength and 1 MAD station (ALS BL5.0.2). All three crystallography end stations have ALS style sample mounters.

Approximately 60% of the users are industrial crystallographers.

**Laboratory experience**

Basic crystallization and sample preparation techniques.

**Other**

Working knowledge of L<sup>A</sup>T<sub>E</sub>X.

Refereed a number of crystallographic papers.

I co-supervise a team of 5 scientific engineering associates at the BCSB.

I supervise a postdoctoral research associate.

## RECENT RESEARCH SUMMARY

I have developed tools that allow users to validate the quality of their experimental crystallographic data. The result is a program named *Xtrriage* which allows the user to obtain an overview of the presence of problems such as twinning, pseudo-translational symmetry, data anisotropy and possible data processing problems. I have furthermore implemented and tested an implementation of refinement against twinned data in *phenix.refine*. Over 40% of structures solved after 2007 that exhibit twinning, are analyzed with the software I developed.

The development of more experimentally oriented methods are focussed on the implementation and optimisation of (semi) automated methods for crystal screening and data collection. This project is related to the efforts related to a *Mail-in* crystallography program currently being organized at the BCSB.

Scientific collaborations involve the structure solution and refinement of a large petidase as well as twinned refinement and pseudo-symmetry properties of a number of crystals. I collaborate with Dr. N.K. Sauter, the author of the Labelit suite, on robust indexing of data sets exhibiting extreme pseudo-translational symmetry as well as nonmerohedral twinning. I collaborate with Prof. Abramson (UCLA) on time resolved Small Angle Scattering Studies of membrane proteins. With Prof. Dr. Read (Cambridge University) I am working on a variety of problems in crystallography, ranging from validation to likelihood based twin refinement.

Besides these project, I am the heading a team that develops the SASTBX, a set of routines for the analyses of Small Angle Scattering data. The SASTBX features data processing, basic analysis,  $P(r)$  estimation, model data generation and structure refinement tools. An alpha release is expected December 2009. The SASTBX currently has tools for fast model-data generation, pair distance distribution function estimation and data reduction. The current emphasis is on model refinement, allowing one to deduce specific structural changes in macromolecules upon ligand binding or change in chemical environment. Due to high ambiguities associated with SAXS data, the use of external restraints derived from biochemical and biophysical experiments as well as data base derived prior information plays in important part in our research.

TEACHING STATEMENT My experiences as an active student in my undergraduate and graduate courses and as a teacher in workshops and conferences have shaped my view on teaching. Being a highly effective teacher is not an easy task to accomplish, but I am of the opinion that a number of key components are of crucial importance.

I view the main task of a teacher to inspire and 'activate' the students to get engaged with the material under review. The result of a good lecture or lecture series should be that the audience grasp the basic concepts taught and, more importantly, have been handed the resources and motivation to go beyond what has been directly taught in class. The way I have tried to accomplish this task during my teaching activities is by including a variety of illustrative real life examples of the topics under study and having other examples ready at hand to illustrate subtleties in a different manner. Another important aspect is to be available for in-depth, one-on-one or small group discussions about the topic, typically during a 'hands on session'.

My main teaching activities have taken place in university group seminars, where I teach and elaborate on highly specialized topics in the field of macromolecular crystallography. I also teach in workshops and conferences (some of which I organized) on more general topics. The overriding philosophy in my teaching is to be flexible and open to suggestions. The interaction with students during group discussions and hands-on sessions, have taught me that the style of teaching and content of the material should be tailored specifically to the audience and their background. I find it furthermore important to receive timely feedback from the students so I can adapt to their specific needs. I accomplish this by talking to students during lecture breaks and having an open door policy afterwards.